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Numerical Simulation of Decoupled Continuous-Time Random Walks with Superheavy-Tailed Waiting Time Distributions

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We develop a numerical method to study the long-time behavior of continuous-time random walks characterized by superheavy-tailed distributions of waiting time. To test the method, we consider symmetric jump-length distributions with both finite second moments and heavy tails for which the asymptotic behavior of the walking particle is known exactly. Our numerical results for the distributions of the particle position are in excellent agreement with the analytical ones.

Keywords: Continuous-time random walks, Superheavy-tailed distributions, Asymptotic behavior, Numerical simulation.

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1. INTRODUCTION

Continuous-time random walks (CTRWs), which were first introduced by Montroll and Weiss [1], represent a powerful and flexible model for the description and analysis of various stochastic systems. Such widespread use of this type of walks is achieved due to the fact that, like the CTRWs, many systems of different nature can be characterized by two random variables, namely, the waiting time between successive jumps and the jump magnitude of the walking particle. The reference walks are especially useful for studying the phenomenon of anomalous diffusion, i.e., diffusion of particles with nonlinear dependence of the mean-square displacement on time [2,3].

One of the most important part of the analysis of the CTRWs is the determination of the asymptotic (in time) behavior of the probability density $P(x,t)$ of the particle position. This problem was already solved for all typical distributions of waiting time and jump magnitude [4,5]. Moreover, its solution was also found for the special but important case of superheavy-tailed waiting time distributions that are characterized by infinite moments of any fractional order [6,7]. It has been recently shown [8] that these CTRWs represent an appropriate tool to describe the phenomenon of superslow diffusion, in which the mean-square displacement grows as a slowly varying function of time.

In the case of typical distributions of waiting time and jump magnitude, which have finite second moments or heavy tails, the numerical determination of $P(x,t)$ at long times can easily be made by the standard methods. But the numerical analysis of the CTRWs with superheavy-tailed distributions of waiting time has some features coming from the absence of finite fractional moments of these distributions and has not been performed before. Therefore, in this paper we develop the numerical method to study the long-time behavior of this type of CTRWs and verify it by comparing the numerical results with the analytical ones obtained in Refs. [6,7].

2. THEORETICAL PART

2.1 Definitions and basic equations

The CTRW is a cumulative continuous-time jump process characterized by a sequence of random jumps of a walking particle. Herewith, the length $x_n \in (-\infty,\infty)$ of the n-th jump is a random variable distributed with probability density $w(x)$, and the waiting time $\tau_n \in [0,\infty)$, i.e., time between $(n$-1)-th and n-th jumps, is a random variable distributed with probability density $p(\tau)$. The particle position $X(t)$ is determined as $X(t) = \sum_{n=1}^{N(t)} x_n$, where $N(t) = 0,1,2,\ldots$ is the number of jumps occurred up to time t (if $N(t) = 0$ then $X(t) = 0$). In the decoupled case, when the sets $\{\tau_n\}$ and $\{x_n\}$ are independent of each other, the probability density $P(x,t)$ of $X(t)$ depends only on the probability densities $p(\tau)$ and $w(x)$. In Fourier-Laplace space this dependence is given by the Montroll-Weiss equation [1]

$$P_{ks} = \frac{1 - p_s}{s(1 - p_s w_k)}, \tag{2.1}$$

where $w_k = \widehat{F}\{w(x)\} = \int_{-\infty}^{\infty} dx\, e^{ikx} w(x)$ $(-\infty < k < \infty)$ is the Fourier transform of the density $w(x)$, $p_s = \widetilde{L}\{p(t)\} = \int_0^\infty dt\, e^{-st} p(t)$ $(\mathrm{Re}\, s > 0)$ is the Laplace transform of the density $p(\tau)$, and $P_{ks} = \widehat{F}\{\widetilde{L}\{P(x,t)\}\}$. Note that since $X(0) = 0$, we have the initial conditions $P(x,0) = \delta(x)$ ($\delta(x)$ is the Dirac δ function) and, because the boundary conditions are not imposed, we get $P(x,t) \to 0$ as $t \to \infty$.

From a more precise point of view, the superheavy-tailed waiting time density $p(\tau)$ and the heavy-tailed jump density $w(x)$, which is assumed to be symmetric, are described by the asymptotic formulas

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$$p(\tau) \sim h(\tau)/\tau \quad (\tau \to \infty)\,, \tag{2.2}$$

$$w(x) \sim u/|x|^{1+\alpha} \quad (|x| \to \infty)\,, \tag{2.3}$$

where the positive function $h(\tau)$ slowly varies at infinity, i.e., $h(\mu\tau) \sim h(\tau)$ as $\tau \to \infty$ for all $\mu > 0$, the tail index α is restricted to the interval $(0,2]$, and u is a positive constant. Note that the difference between the asymptotic formulas (2.2) and (2.3) causes the difference between the fractional moments of $p(\tau)$ and $w(x)$. Specifically, while the fractional moments $\int_0^\infty d\tau\, \tau^\rho p(\tau)$ of $p(\tau)$ are infinite for all $\rho > 0$, the fractional moments $\int_{-\infty}^\infty dx |x|^\rho w(x)$ of $w(x)$ are infinite only if $\rho \geq \alpha$. Therefore, the variance of $w(x)$ is infinite for all jump densities with $\alpha \in (0,2]$. We note also that, due to the normalization condition $\int_0^\infty d\tau\, p(\tau) = 1$, the slowly varying function $h(\tau)$ must possess the following property: $h(\tau) = o(1/\ln\tau)$ as $\tau \to \infty$.

2.2 Previous analytical results

In this subsection we briefly outline the main theoretical results obtained in Refs. [6,7] and which we are going to verify in Sec. 3 using numerical simulation. Since the probability density of walker position vanishes at long times, $P(x,t) \to 0$ as $t \to \infty$, it is reasonable to introduce a new scaled walker position $Y(t) = a(t)X(t)$, where $a(t)$ is a positive scaling function, whose probability density $P(y,t)$ is nonvanishing and nondegenerate. Using the relation $P(x,t)dx = P(y,t)dy$, one can get the limiting probability density of a properly scaled walker position $Y(t)$

$$\mathrm{P}(y) = \lim_{t\to\infty} a^{-1}(t) P(a^{-1}(t)y, t)\,. \tag{2.4}$$

According to this, the asymptotic behavior of the original probability density $P(x,t)$ at $t \to \infty$ is given by

$$P(x,t) \sim a(t)\,\mathrm{P}(a(t)x)\,. \tag{2.5}$$

It has been shown [6] that in the case of superheavy-tailed waiting time distributions and jump-length distributions with finite second moments the limiting probability density and the corresponding scaling function at $t \to \infty$ can be represented as

$$\mathrm{P}(y) = \frac{1}{2} e^{-|y|} \tag{2.6}$$

and

$$a(t) \sim \sqrt{2V(t)/l_2}\,, \tag{2.7}$$

respectively. Here, $V(t) = \int_t^\infty d\tau\, p(\tau)$ is the so-called survival or exceedance probability, i.e., the probability that up to time t the walking particle remains at the origin, and $l_2 = \int_{-\infty}^\infty dx x^2 w(x)$ is the second moment of the jump density $w(x)$.

In contrast, if the jump-length distributions are heavy-tailed, then, according to [7],

$$\mathrm{P}(y) = \frac{1}{\pi} \int_0^\infty dx \frac{\cos(yx)}{1 + x^\alpha} \tag{2.8}$$

with $\alpha \in (0,2]$ and

$$a(t) \sim \left[\frac{\Gamma(1+\alpha)\sin(\pi\alpha/2)}{\pi u} V(t) \right]^{1/\alpha} \tag{2.9}$$

with $\alpha \in (0,2)$. At $\alpha = 2$ Eq. (2.8) reduces to Eq. (2.6), but the scaling function in this case differs from that given in Eq. (2.7):

$$a(t) \sim \sqrt{\frac{2V(t)}{u \ln V^{-1}(t)}}\,. \tag{2.10}$$

It should be noted that the limiting density (2.8) can also be represented in the form

$$\mathrm{P}(y) = \frac{1}{\pi} \int_0^\infty dx\, e^{-|y|x} \frac{\sin(\pi\alpha/2) x^\alpha}{1 + 2\cos(\pi\alpha/2) x^\alpha + x^{2\alpha}}\,. \tag{2.11}$$

This representation is more preferable for studying the general properties of $\mathrm{P}(y)$. In particular, from Eq. (2.11) immediately follows [in contrast to Eq. (2.8)] that $\mathrm{P}(y)$ is positive and unimodal. We note also that the symmetry property $\mathrm{P}(-y) = \mathrm{P}(y)$ is a consequence of the condition $w(-y) = w(y)$, which is assumed to hold. One more important feature of the limiting density, which takes place if $\alpha \in (0,2)$, is that it is a heavy-tailed function with the same tail index α characterizing the asymptotic behavior of $w(x)$. However, although the jump-length density $w(x)$ at $\alpha = 2$ is still heavy-tailed, in this case the tails of $\mathrm{P}(y)$ are exponential. Finally, we stress that, because of the superheavy-tailed character of $p(t)$, in both cases, when $w(x)$ has finite second moment or heavy tails, the scaling functions $a(t)$ vary slowly at infinity. Therefore, in accordance with Eq. (2.5), the long-time evolution of the probability density $P(x,t)$ occurs very slowly.

3. NUMERICAL SIMULATIONS

3.1 Algorithm

Since we are going to numerically study the long-time behavior of the walking particle with large waiting times, the observation time interval $[0, T]$ should be chosen as large as possible. According to the definition, the particle starts to walk at time $t = 0$ from the position $X(0) = 0$. After (random) waiting time τ_1 the particle makes a jump of length x_1 and at $t = \tau_1$ its new position becomes $X(\tau_1) = x_1$. Then, after next waiting time τ_2 the particle makes a jump of length x_2 occupying at $t = \tau_1 + \tau_2$ the position $X(\tau_1 + \tau_2) = x_1 + x_2$, and so on. Now, let us assume that during the time $t = T$ exactly N jumps occurred (i.e., $\sum_{n=1}^N \tau_n \leq T$ and $\sum_{n=1}^{N+1} \tau_n > T$). In this case the particle position at $t = T$ is determined as $X(T) = \sum_{n=1}^N x_n$. Because we are interested in numerical finding the limiting probability densities, it is reasonable to use the scaled particle position $Y(T)=a(T)X(T)$ with the scaling function $a(T)$ taken from Eq. (2.7), (2.9) or (2.10) depending on the character of the walk. Calculating the random variable $Y(T)$ many times, one can evaluate its distribution, which is associated with the limiting one.

Since the waiting times τ_n and jump magnitudes x_n are distributed with some probability densities $p(\tau)$ and $w(x)$, the method of their generation should be introduced. There are many such methods [9], but here we employ the inverse one that uses the fact that every strictly increasing distribution function has the inverse function. This method is based on the theorem, which states that if $F(\xi)=\int_{-\infty}^{\xi} d\xi' f(\xi')$ is a continuous distribution function and $F^{-1}(U)=\inf\{\xi : F(\xi)=U, 0<U<1\}$ is its inverse function, then $\xi=F^{-1}(U)$ with U being a uniform random variable on (0,1) has the cumulative distribution function $F(\xi)$. Thus, if the probability densities $p(\tau)$ and $w(x)$ are positive, then the distribution functions $\Phi(\tau)=\int_0^{\tau} d\tau' p(\tau')$ and $\Psi(x)=\int_{-\infty}^{x} dx' w(x')$ can be inverted, and so the waiting times and jump magnitudes can be determined by the inverse method.

Using the above, we introduce the following algorithm for the numerical simulation of the scaled particle position $Y(T)$:

```
The initial position: X ← 0
The initial time: t ← 0
The walking time: T
REPEAT
   Generate a random variable U uniformly distributed on (0,1)
   Calculate waiting time τ ← Φ^{-1}(U)
   Calculate waking time t ← t + τ
   IF t ≤ T
      THEN
         Generate a random variable U* uniformly distributed on (0,1)
         Calculate jump magnitude x ← Ψ^{-1}(U*)
         Calculate particle position X ← X + x
      ELSE
         Calculate a(T) from Eq. (2.7), (2.9) or (2.10)
         RETURN scaling position Y = a(T)X
UNTIL t ≤ T
```

It is important to emphasize that the proposed algorithm can easily be extended to the CTRWs in a multidimensional space and with coupled sets $\{\tau_n\}$ and $\{x_n\}$.

3.2 Examples

To apply the above algorithm, we should know the probability densities $p(\tau)$ and $w(x)$. For the illustrative purposes of this paper, it is convenient to choose these densities in the simplest form in order to obtain the waiting times and jump magnitudes analytically. In particular, the superheavy-tailed probability density of waiting times can be chosen in the following form:

$$p(\tau)=\frac{\gamma \ln^{\gamma}\eta}{(\eta+\tau)\ln^{\gamma+1}(\eta+\tau)} \qquad (3.1)$$

($\eta>1$, $\gamma>0$). In this case the waiting times are determined as $\tau_n=\eta^{(1-U_n)^{-1/\gamma}}-\eta$, where U_n are random numbers uniformly distributed in the interval (0,1). On average, these times strongly increase with decreasing the parameter γ. Therefore, to save the computing time and memory, it is reasonable to put $\gamma>1$.

To test the numerical method for the jump-length densities with different asymptotic behavior, we considered two cases. They are represented by the Gaussian density

$$w(x)=\frac{e^{-x^2/2}}{\sqrt{2\pi}} \qquad (3.2)$$

with the finite second moment and the heavy-tailed density

$$w(x)=\frac{rb^r}{2(b+|x|)^{1+r}} \qquad (3.3)$$

($b>0$, $r\in(0,2]$) with the tail index $\alpha=r$. The jump magnitudes that correspond to the probability densities (3.2) and (3.3) are given by $x_n=\sqrt{2}\,\mathrm{erf}^{-1}(2U_n^*-1)$ [$\mathrm{erf}^{-1}(x)$ is the inverse error function, U_n^* are random numbers uniformly distributed in the interval (0,1)] and $x_n=(\pm)_n b[(1-U_n^*)^{-1/r}-1]$ [$(\pm)_n=+1$ or -1 with probability 1/2 each], respectively. In Fig. 1 we show the limiting probability densities, which correspond to the above waiting-time and jump-length densities, calculated by Eqs. (2.6) and (2.11) (solid and dashed lines) and by numerical simulations (symbols).

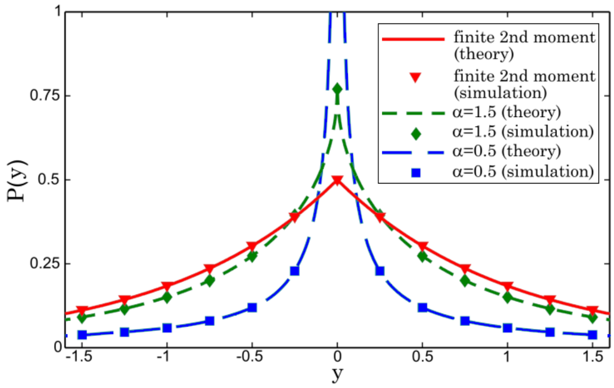

Fig. 1 – Theoretical and simulated limiting probability densities in particular cases. In all these cases the waiting-time density is given by Eq. (3.1) with $\gamma=4, \eta=2$. The jump-length densities are taken from Eq. (3.2) (red solid lines and triangles) and from Eq. (3.3) with $r=3/2, b=1$ (green short-dashed lines and diamonds) and $r=1/2, b=1$ (blue long-dashed lines and squares). The walking time equals $T=10^{25}$ and the number of particles (runs) equals 10^6

As clearly seen from this figure, the simulated results are in full agreement with the theoretical ones.

Finally, to demonstrate the efficiency of the proposed method in higher dimensions, we performed simulations of trajectories of a walking particle in a two-dimensional space. As before, we assume that the waiting-time distributions are superheavy-tailed, but now the jump-length distributions are considered to be two-dimensional and characterized by a joint probability density $w(x, y)$. If the jumps along the axes x and y are statistically independent and distributed with the same probability density then $w(x, y) = w(x)w(y)$. For illustration, in Figs. 2 and 3 we show the sample trajectories that correspond to two CTRWs with different distributions of waiting time and jump magnitude. In both cases the jumps are assumed to be independent, but in Fig. 2 they are distributed with the Cauchy distribution and in Fig. 3 with the Gaussian distribution. The difference between these trajectories arises from that the asymptotic behaviors of $p(\tau)$ and $w(x)$ in these cases are different. Indeed, at the same other conditions, the slower $p(\tau)$ decays as $\tau \to \infty$, the smaller the number of jumps is. Similarly, the slower $w(x)$ decays as $|x| \to \infty$, the larger the trajectory domain is.

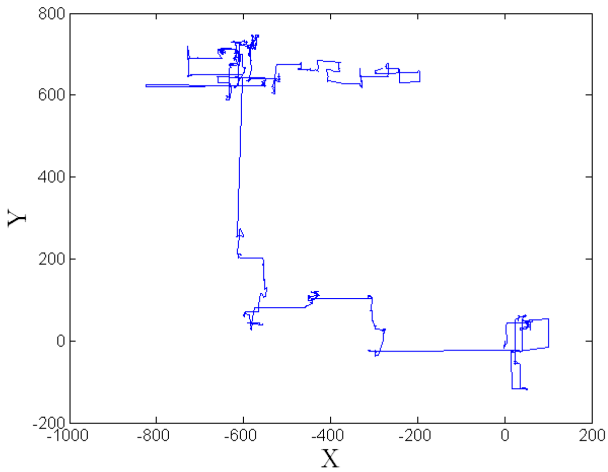

Fig. 2 – Sample trajectory of a walking particle. The waiting-time density is determined by Eq. (3.1) with $\gamma = 4, \eta = 2$ and the joint probability density of jump magnitudes is given by $w(x, y) = \pi^{-2}(1 + x^2)^{-1}(1 + y^2)^{-1}$. For this illustrative example, the particle has made about 700 jumps during the time $t = 10^3$

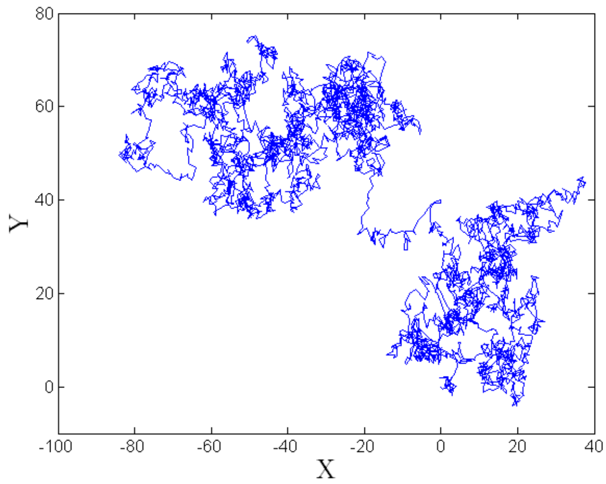

Fig. 3 – Sample trajectory of a walking particle. The waiting-time density is determined by Eq. (3.1) with $\gamma = 8, \eta = 2$ and the joint probability density of jump magnitudes is given by $w(x, y) = (2\pi)^{-1} e^{-(x^2+y^2)/2}$. For this illustrative example, the particle has made about 5200 jumps during the time $t = 10^3$

4. CONCLUSIONS

We have developed a numerical algorithm to study the long-time behavior of the continuous-time random walks (CTRWs) characterized by superheavy-tailed distributions of waiting time. In order to examine the proposed method and verify the previously obtained analytical results, we have calculated the limiting probability densities of the walker position in some particular cases and have compared them with the analytical ones. These cases include examples of CTRWs with a certain superheavy-tailed distribution of waiting time and three jump-length distributions, one of which has a finite second moment and the others heavy tails. It is shown that the numerical method correctly reproduces analytical results and is an efficient tool for the investigation of a given class of CTRWs in a space of arbitrary dimension.

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